

(FILE 'HOME' ENTERED AT 22:19:27 ON 19 SEP 2003)

FILE 'REGISTRY' ENTERED AT 22:19:48 ON 19 SEP 2003
L1 STRUCTURE uploaded

=> d 11
L1 HAS NO ANSWERS
L1 STR

Structure diagram not available for display

Structure attributes must be viewed using STN Express query preparation.

=> s 11
SAMPLE SEARCH INITIATED 22:20:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 543 TO ITERATE

100.0% PROCESSED 543 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9462 TO 12258
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full
FULL SEARCH INITIATED 22:20:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 10590 TO ITERATE

100.0% PROCESSED 10590 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.03

L3 24 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS SINCE FILE TOTAL
FULL ESTIMATED COST ENTRY SESSION
148.55 148.76

FILE 'CAPLUS' ENTERED AT 22:20:50 ON 19 SEP 2003
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FILE COVERS 1907 - 19 Sep 2003 VOL 139 ISS 13
FILE LAST UPDATED: 18 Sep 2003 (20030918/ED)

This file contains CAS Registry Numbers for easy and accurate

substance identification.

=> s 13
L4 13 L3

=> d 1-13 bib abs

L4 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:741154 CAPLUS
DN 137:384890
TI Density Functional Theory Studies of Titanium-Catalyzed Hydroboration of Olefins
AU Liu, Dan; Lin, Zhenyang
CS Institute of Molecular Technology for Drug Discovery and Synthesis, Department of Chemistry and Open Laboratory of Chirotechnology, Hong Kong University of Science and Technology, Kowloon, Hong Kong, Peop. Rep. China
SO Organometallics (2002), 21(22), 4750-4755
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB The B3LYP method of d. functional theory is used to study the hydroboration reaction of olefins catalyzed by Cp2Ti(HBcat'). The favorable pathway is where the active species Cp2Ti(HBcat') initially coordinates an olefin to form a structural intermediate having a five-membered ring with a Ti-H-B bridging unit. B-H bond cleavage then occurs to allow the reductive elimination to form alkylboronate ester as the main product. Calcs. show that from the B-H cleavage species the .beta.-hydride elimination leading to the formation of side products, vinylboronate ester, is also competitive. Ti-O coordination is the main reason for the lowering of the barrier of reductive elimination to form the main product, alkylboronate ester. The related olefin hydrogenation process has also been studied.

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:574273 CAPLUS
DN 133:252528
TI Measurement of Barriers for Alkene Dissociation and for Inversion at Zirconium in a d0 Zirconium-Alkyl-Alkene Complex
AU Casey, Charles P.; Carpenetti, Donald W., II
CS Department of Chemistry, University of Wisconsin, Madison, WI, 53706, USA
SO Organometallics (2000), 19(19), 3970-3977
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB The .beta.-allyl zirconacyclobutane complex Cp*2Zr[CH2CH(CH2CH:CH2)CH2] (7) reacted rapidly with B(C6F5)3 in CD2Cl2 at -78.degree. to form the zwitterionic d0 zirconium(IV) chelate complex Cp*2Zr[.eta.1,.eta.2-CH2CH[CH2B(C6F5)3]CH2CH:CH2] (2a and 2b). Low-temp. 1H, 13C, TOCSY1D, and NOESY1D NMR spectroscopy of 2 established the bonding of the tethered alkene to the d0 metal center. A dynamic NMR study of the interconversion of 2a and 2b allowed measurement of the alkene dissociation energy (.DELTA.G.thermod. = 10.5 (2a to 2b) and 10.3 (2b to 2a) kcal mol-1), but the complex decompd. before the barrier for site epimerization at the zirconium center could be detd. Reaction of 7 with [(C6H5)2(CH3)NH][B(C6F5)4] led to the formation of two isomeric d0 zirconium(IV)-alkyl-alkene chelates Cp*2Zr[.eta.1,.eta.2-CH2CH(CH3)CH2CH:CH2][B(C6F5)4] (8a and 8b). This more thermally stable zirconium-alkyl-alkene complex allowed the measurement of barriers assocd. with decomplexation of the alkene (.DELTA.G.thermod. = 10.7 and 11.1 kcal

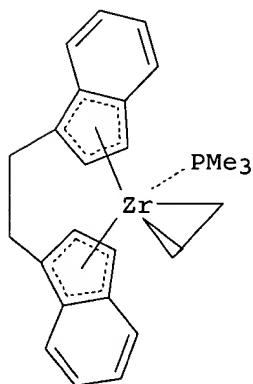
mol-1) and site epimerization at the zirconium center (.DELTA.G.thermod. = 14.4 kcal mol-1) by line shape anal. of variable-temp. 1H and 13C NMR spectra.

RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:629438 CAPLUS
DN 131:351709
TI Observation of Zwitterionic d0 Zirconium-Alkyl-Alkene Chelates: Models for Intermediates in Metallocene-Catalyzed Alkene Polymerizations
AU Casey, Charles P.; Carpenetti, Donald W., II; Sakurai, Hidehiro
CS Department of Chemistry, University of Wisconsin, Madison, WI, 53706, USA
SO Journal of the American Chemical Society (1999), 121(40), 9483-9484
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB The reaction of Stryker's .beta.-allyl zirconacyclobutane complex Cp*2Zr[CH2CH(CH2CH:CH2)CH2] (I) with B(C6F5)3 at -78.degree. in CD2Cl2 led to the formation of a bright orange soln. contg. two isomers of Cp*2Zr+ [.eta.1,.eta.2-CH2CH[CH2B-(C6F5)3]CH2CH:CH2]. The 1H and 13C NMR spectra at -82.degree. showed the presence of a 1.8:1 mixt. of two diastereomers of the zwitterionic d0 zirconium(IV) chelate complex. Evidence of alkene complexation came from perturbation of the vinyl hydrogen chem. shifts compared with those of I.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

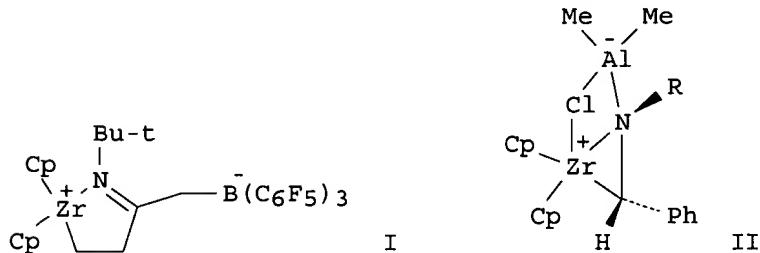
L4 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:522457 CAPLUS
DN 131:271962
TI Zwitterionic Metallocenes Derived from rac and meso-Ethylenebisindenyl Zirconocene Olefin Complexes and Pentafluorophenyl-Substituted Boranes
AU Lee, Lawrence W. M.; Piers, Warren E.; Parvez, Masood; Rettig, Steven J.; Young, Victor G., Jr.
CS Department of Chemistry, University of Calgary, Calgary, AB, T2N 1N4, Can.
SO Organometallics (1999), 18(19), 3904-3912
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:271962
GI



AB Trimethylphosphine-stabilized ethylene complexes, e.g. I, of the ethylenebisindenyl-supported zirconocene fragment are prep'd. via magnesium redn. of rac-(EBI)ZrCl₂ in the presence of ethylene and PMe₃. When the reaction is halted after 6 h, good yields of a mixt. contg. rac-(EBI)Zr(.eta.2-CH₂:CH₂)PMe₃, rac-1, and the racemic diastereomer of the zirconacyclopentane deriv. (EBI)Zr(.eta.2-CH₂CH₂CH₂CH₂), rac-2, are obtained. This mixt. may be converted to pure rac-1 if treated with excess PMe₃. If the magnesium redn. of rac-(EBI)ZrCl₂ is left for 3 days in the presence of magnesium chloride, complete epimerization to meso-1 is obsd. Thus, both diastereomers of 1 are available. Compds. meso-1 and rac-2 have been characterized crystallog. The coordinated ethylene ligands in compds. 1 are susceptible to electrophilic attack by the pentafluorophenyl-substituted boranes HB(C₆F₅)₂ and B(C₆F₅)₃, forming zwitterionic metallocene products. For reactions involving HB(C₆F₅)₂, the products meso-3 and rac-3 are characterized by a strong zirconium-hydrido borate interaction, as well as a weak Zr-C.beta. bonding. In addn. to complete soln. characterization, the structure of meso-3 was detd. crystallog. Upon treatment of rac-1 with B(C₆F₅)₃, a more charge-sepd. zwitterion, rac-4, was formed. In addn. to retaining its PMe₃ ligand, the complex is stabilized by a strong .beta.-CH₂ interaction, as detd. by x-ray crystallog. and NMR spectroscopy. Structural comparisons between the compds. reported herein and previous examples in metallocene chem. are presented.

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:516548 CAPLUS
DN 131:271961
TI Reaction of the Lewis Acids B(C₆F₅)₃ and (AlMe₂Cl)₂ with Azazirconacycles
AU Harlan, C. Jeff; Bridgewater, Brian M.; Hascall, Tony; Norton, Jack R.
CS Department of Chemistry, Columbia University, New York, NY, 10027, USA
SO Organometallics (1999), 18(19), 3827-3834
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:271961
GI

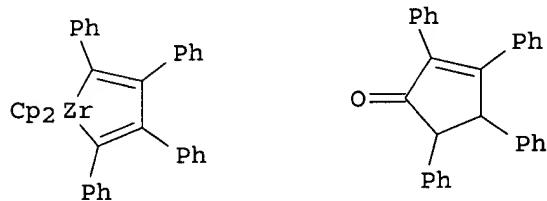


AB B(C₆F₅)₃ opens the ring of the N-tBu azazirconacyclobutane Cp₂Zr(N(tBu)CH₂CH₂-C,N) by abstracting the C from the Zr; the resulting amido cation Cp₂Zr(N(tBu)CH₂CH₂B(C₆F₅)₃) reacts slowly with ethylene to form a chelating .gamma.-iminoalkyl zirconocene cation Cp₂Zr(N(tBu):C(CH₂B(C₆F₅)₃)CH₂CH₂-C,N) (4; shown as I). Similarly, B(C₆F₅)₃ removes C from the Zr of the N-Ph azazirconacyclopentane 5a (Cp₂Zr(NPhCHPhCH₂CH₂-C,N)) and the N-SiMe₃ azazirconacyclopentane 5b (Cp₂Zr(N(SiMe₃)CHPhCH₂CH₂-C,N)), forming amido cations that are stabilized in the solid state by coordination of Ph substituents on N (6, from 5a) or C (8, from 5b). 8 Slowly loses H, forming an azaallyl cation

Cp₂Zr(.eta.3-N(SiMe₃)CPhCHCH₂B(C₆F₅)₃). In contrast AlMe₂Cl coordinates the N of the zirconiaaziridines Cp₂Zr(THF)(NRCHPh-C,N) (R = Ph, SiMe₃), resulting in an sp₂ N coordinated to Zr through a p orbital in Cp₂Zr(N(AlMe₂Cl)(R)CPh-C,N) (11; shown as II). The structures of 4, 6, 8, and 11a were established by x-ray crystallog.

RE.CNT 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:44179 CAPLUS
DN 130:209779
TI Reaction of Zirconacyclopentadienes with CO in the Presence of n-BuLi.
Selective Formation of Cyclopentenone Derivatives from Two Alkynes and CO
AU Takahashi, Tamotsu; Huo, Shouquan; Hara, Ryuichiro; Noguchi, Yoshinori;
Nakajima, Kiyohiko; Sun, Wen-Hua
CS Catalysis Research Center and Graduate School of Pharmaceutical Sciences,
Hokkaido University, Sapporo, 060, Japan
SO Journal of the American Chemical Society (1999), 121(5), 1094-1095
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
OS CASREACT 130:209779
GI



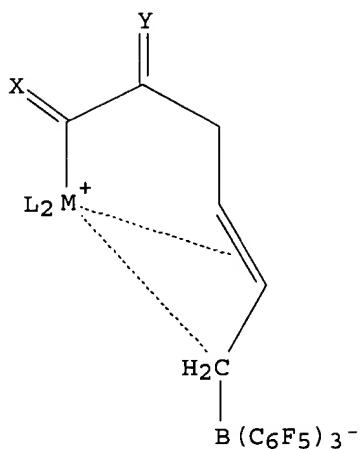
I

II

AB The title reaction is described. Thus, reaction of zirconacyclopentadiene I with BuLi followed by treatment with CO gave 80% cyclopentenone II as a mixt. of cis and trans isomers. The crystal structure of trans-II was detd.

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1997:564531 CAPLUS
DN 127:262793
TI Evidence for internal ion-pair formation upon insertion of reactive alkenes in the zirconium-carbon bond of the Cp₂Zr(.nu.-C₄H₆)B(C₆F₅)₃ metallocene-boron-betaine Ziegler catalyst system
AU Karl, Jorn; Erker, Gerhard
CS Organisch-Chemisches-Institut, Universitat Munster, Muenster, D-48149, Germany
SO Chemische Berichte/Recueil (1997), 130(9), 1261-1267
CODEN: CHBRFW
PB Wiley-VCH
DT Journal
LA English
OS CASREACT 127:262793
GI



I

AB Treatment of the (butadiene)ML2 complexes [ML2 = Cp2Zr, Cp2Hf, (.eta.-C5H4Me)2Zr; Cp = cyclopentadienyl] with B(C6F5)3 gives the 1:1 adducts [CH2:CHCH:CH2B(C6F5)3]ML2. At -40.degree., the betaine complex [CH2:CHCH:CH2B(C6F5)3]ZrCp2 inserts 1 equiv. methylenecyclopropane to give the regioisomeric insertion products I [M = Zr; L = Cp; X = H2, Y = (CH2)2 or X = (CH2)2, Y = H2] in a 60:40 ratio. These products exhibit the cyclopropylidene moiety in the .alpha.- and .beta.-positions, resp., relative to Zr. The corresponding Hf complexes are obtained in a 70:30 ratio starting from [CH2:CHCH:CH2B(C6F5)3]HfCp2. The reaction of [CH2:CHCH:CH2B(C6F5)3]ML2 with allene gives a single insertion product in each case where the exo-methylene group is in the .alpha.-position to the metal center ([2,1]-insertion). The new complexes are chiral. They all exhibit a pronounced .pi.-interaction of the internal C(4)H:C(5)H double bond of the .sigma.-ligand chain with the metal center in addn. to a metallocene/C(6)H2[B] ion pair interaction. The relative contributions of these 2 components to the intramol. stabilization of the cationic metallocene end of the dipolar complexes are dependent on the steric and electronic properties of the resp. metallocene units involved. This is revealed by a comparison of typical 13C-NMR parameters of the complexes with a pair of suitable model complexes, namely the ethylene insertion product into the betaine system [CH2:CHCH:CH2B(C6F5)3]ZrCp2 and its THF adduct.

L4 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1996:170744 CAPLUS
 DN 124:203315
 TI Zwitterionic transition metal compounds, their preparation and use as olefin polymerization catalysts
 IN Erker, Gerhard; Temme, Bodo; Aulbach, Michael; Bachmann, Bernd; Kueber, Frank
 PA Hoechst A.-G., Germany
 SO Ger. Offen., 10 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	-----	-----	-----	-----
PI DE 4420456	A1	19951214	DE 1994-4420456	19940613

AU 9520278	A1	19951221	AU 1995-20278	19950524
AU 691589	B2	19980521		
EP 687682	A1	19951220	EP 1995-108411	19950601
EP 687682	B1	20000119		
R: AT, BE, DE, ES, FR, GB, IT, NL, SE				
EP 992516	A2	20000412	EP 1999-110599	19950601
EP 992516	A3	20021030		
R: AT, BE, DE, ES, FR, GB, IT, NL, SE				
ES 2142426	T3	20000416	ES 1995-108411	19950601
TW 387905	B	20000421	TW 1995-84105602	19950605
US 5792819	A	19980811	US 1995-475940	19950607
US 6002032	A	19991214	US 1995-478900	19950607
FI 9502857	A	19951214	FI 1995-2857	19950609
RU 2140922	C1	19991110	RU 1995-109885	19950609
CA 2151558	AA	19951214	CA 1995-2151558	19950612
NO 9502307	A	19951214	NO 1995-2307	19950612
ZA 9504829	A	19960130	ZA 1995-4829	19950612
BR 9502776	A	19960312	BR 1995-2776	19950612
JP 08003212	A2	19960109	JP 1995-145881	19950613
CN 1119648	A	19960403	CN 1995-107172	19950613
CN 1069646	B	20010815		

PRAI DE 1994-4420456 A 19940613
 EP 1995-108411 A3 19950601

OS MARPAT 124:203315

AB The zwitterionic compds. LnM+YZA-Rm [A = Group IB, IIB, III, IVA, V, VIB, VIIIB, or VIIIB element; each L = pi -bonded ligand, electron donor (2 L may be joined by a bridging group); M = Group III-VI transition metal; each R = perhalocarbyl; Y = hetero atom, hydrocarbon residue; Z = hydrocarbon residue; m = 1-5, n = 1-4] are prep'd. by reaction of LnMX_2 (X = halogen) with YZ_2^- , followed by treatment with ARM . Thus, [(dimethylsilylene)bis(2-methyl-4,5-benzindenyl)]zirconium dichloride and (2-butene-1,4-diyl)magnesium-2THF were stirred in toluene at -40.degree. and allowed to warm to room temp., filtered, and evapd. to dryness to give a red powder, which was redissolved in toluene and treated with tris(pentafluorophenyl)borane to give a zwitterion $\text{L}_2\text{Zr+CH}_2\text{CH:CHCH}_2\text{B-}$ (C_6F_5)₃, where L2 is the bridged bis(benzindenyl) ligand. This zwitterion, formed in situ, was used with iso-Bu₃Al to polymerize propylene, giving isotactic polypropylene with wt.-av. mol. wt. 298,000 and polydispersity 2.2. Other related zwitterions produced syndiotactic polypropylene.

L4 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1977:552744 CAPLUS
 DN 87:152744
 TI Polyethylene
 IN Sinn, Hansjoerg; Mottweiler, Renke; Andresen, Arne; Cordes, Hans Guenther; Herwig, Jens; Kaminsky, Walter; Merck, Alexander; Vollmer, Hans Juergen; Pein, Joachim
 PA BASF A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 10 pp.

CODEN: GWXXBX

DT Patent
 LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	-----	-----	-----	-----
PI	DE 2608933	A1	19770908	DE 1976-2608933	19760304
	DE 2608933	C2	19890706		

PRAI DE 1976-2608933 19760304

AB Ziegler catalysts are prep'd. from cyclopentadienyl Zr compds. and Et₃Al [97-93-8] (1:0.001-20 mole ratio) for the manuf. of polyethylene (I) [9002-88-4] at -80 to +120.degree.. The catalysts are halogen-free and, optionally, may contain H₂O for mol. wt. regulation. Thus, 0.1 mol tetrakis(cyclopentadienyl)zirconium [1273-01-4] was mixed with 0.7 mol

Et₃Al at 60.degree. until ethane evolution ceased (.apprx.1 wk) to give a dark red oil which was dild. to 300 mL with heptane. The catalyst (0.0022 mol/L Zr) was added to a reactor contg. 300 mL C₆H₆, the mixt. heated to 50.degree., and ethylene (9 bar) fed in. After 64 h, I yield was 81 g/L and the mol. wt. was 1,500,000.

L4 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1976:576721 CAPLUS
DN 85:176721
TI Extremely strained bond angle in organozirconium compounds which are active with respect to ethylene
AU Kaminsky, Walter; Kopf, Juergen; Sinn, Hansjoerg; Vollmer, Hans J.
CS Inst. Anorg. Angew. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SO Angewandte Chemie (1976), 88(20), 688-9
CODEN: ANCEAD; ISSN: 0044-8249
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB The ZrCH₂CH bond angle in I and II was detd. via x-ray anal. to be .apprx.76.degree.. The cyclopentadiene anion in II is positioned between two neighboring Zr centers.

L4 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1975:458968 CAPLUS
DN 83:58968
TI Ethanes bearing several metal substituents
AU Kaminsky, Walter; Sinn, Hansjoerg
CS Inst. Anorg. Angew. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SO Justus Liebigs Annalen der Chemie (1975), (3), 424-37
CODEN: JLACBF; ISSN: 0075-4617
DT Journal
LA German
GI For diagram(s), see printed CA Issue.
AB Cp₂ZrCl₂ (Cp = .pi.-cyclopentadienyl) and Et₃Al gave Cp₂ZrEtCl, which with Et₃Al gave I, which eliminated Et to give II. II on treatment with THF lost 2 Et₃Al·THF to give Cp₂ZrClCH₂CH₂ZrClCp₂. I also eliminated Et to give Cp₂ZrClCH₂CH₂AlEt₂ which reacted with AlEt₃ to give Cp₂ZrClCH₂CH(AEt₂)₂ (III). III reacted with AlEt₃ to give Cp₂ZrEtCH₂CH(AEt₃)₂ and Et₂AlCH₂CH₂ZrCp₂CH₂CH(AEt₃)₂. The latter with AlEt₃ gave [(Et₂Al)₂CHCH₂]₂ZrCp₂ and IV and V.

L4 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1975:435365 CAPLUS
DN 83:35365
TI Nuclear magnetic resonance investigations on dicyclopentadienylzirconium(I V) and organoaluminum systems
AU Kaminsky, Walter; Vollmer, Hans J.
CS Inst. Anorg. Angew. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SO Justus Liebigs Annalen der Chemie (1975), (3), 438-48
CODEN: JLACBF; ISSN: 0075-4617
DT Journal
LA German
AB The PMR spectra were recorded of complexes formed from Et₂Zr(cp)₂Cl and Et₃Al (cp = cyclopentadienyl) and their deuterated analogs. Coalescence temps., structures, conformations, and bonding are discussed.

L4 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1974:490758 CAPLUS
DN 81:90758
TI Formation of dimetallocalkylenes, an inevitable secondary reaction of homogeneous Ziegler catalysts
AU Kaminsky, Walter; Vollmer, Hans J.; Heins, Erhard; Sinn, Hansjoerg
CS Inst. Anorg. Angew. Chem., Univ. Hamburg, Hamburg, Fed. Rep. Ger.
SO Makromolekulare Chemie (1974), 175(2), 443-56

CODEN: MACEAK; ISSN: 0025-116X
DT Journal
LA German
AB Homogeneous Ziegler catalysts, e.g., Cp2ZrCl2-AlEt3 (Cp = cyclopentadienyl), undergo β -H transfer with condensation and alkane cleavage to give dimetallocalkylenes, e.g., Cp2ZrClCH2CH2AlEt2. The mechanism and structures are based on kinetic data, NMR measurements, quenching techniques with DCl, and material balances.

=> s 14 and zwitterionic
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L5 4 L4 AND ZWITTERIONIC

=> d 1-4 bib abs

L5 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:574273 CAPLUS
DN 133:252528
TI Measurement of Barriers for Alkene Dissociation and for Inversion at Zirconium in a d0 Zirconium-Alkyl-Alkene Complex
AU Casey, Charles P.; Carpenetti, Donald W., II
CS Department of Chemistry, University of Wisconsin, Madison, WI, 53706, USA
SO Organometallics (2000), 19(19), 3970-3977
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
AB The β -allyl zirconacyclobutane complex Cp*2Zr[CH2CH(CH2CH:CH2)CH2] (7) reacted rapidly with B(C6F5)3 in CD2Cl2 at -78.degree. to form the zwitterionic d0 zirconium(IV) chelate complex Cp*2Zr[.eta.1,.eta.2-CH2CH[CH2B(C6F5)3]CH2CH:CH2] (2a and 2b). Low-temp. 1H, 13C, TOCSY1D, and NOESY1D NMR spectroscopy of 2 established the bonding of the tethered alkene to the d0 metal center. A dynamic NMR study of the interconversion of 2a and 2b allowed measurement of the alkene dissociation energy ($\Delta G_{thermod.}$ = 10.5 (2a to 2b) and 10.3 (2b to 2a) kcal mol-1), but the complex decompd. before the barrier for site epimerization at the zirconium center could be detd. Reaction of 7 with [(C6H5)2(CH3)NH]B(C6F5)4 led to the formation of two isomeric d0 zirconium(IV)-alkyl-alkene chelates Cp*2Zr[.eta.1,.eta.2-CH2CH(CH3)CH2CH:CH2]B(C6F5)4 (8a and 8b). This more thermally stable zirconium-alkyl-alkene complex allowed the measurement of barriers assocd. with decomplexation of the alkene ($\Delta G_{thermod.}$ = 10.7 and 11.1 kcal mol-1) and site epimerization at the zirconium center ($\Delta G_{thermod.}$ = 14.4 kcal mol-1) by line shape anal. of variable-temp. 1H and 13C NMR spectra.

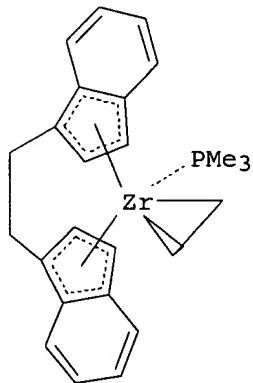
RE.CNT 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:629438 CAPLUS
DN 131:351709
TI Observation of Zwitterionic d0 Zirconium-Alkyl-Alkene Chelates: Models for Intermediates in Metallocene-Catalyzed Alkene Polymerizations
AU Casey, Charles P.; Carpenetti, Donald W., II; Sakurai, Hidehiro
CS Department of Chemistry, University of Wisconsin, Madison, WI, 53706, USA
SO Journal of the American Chemical Society (1999), 121(40), 9483-9484
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
AB The reaction of Stryker's β -allyl zirconacyclobutane complex Cp*2Zr[CH2CH(CH2CH:CH2)CH2] (I) with B(C6F5)3 at -78.degree. in CD2Cl2 led to the formation of a bright orange soln. contg. two isomers of

$Cp^*Zr[\eta.1,\eta.2-CH_2CH[CH_2B-(C_6F_5)_3]CH_2CH:CH_2]$. The 1H and ^{13}C NMR spectra at -82.degree. showed the presence of a 1.8:1 mixt. of two diastereomers of the zwitterionic d0 zirconium(IV) chelate complex. Evidence of alkene complexation came from perturbation of the vinyl hydrogen chem. shifts compared with those of I.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:522457 CAPLUS
DN 131:271962
TI Zwitterionic Metallocenes Derived from rac and meso-Ethylenebisindenyl Zirconocene Olefin Complexes and Pentafluorophenyl-Substituted Boranes
AU Lee, Lawrence W. M.; Piers, Warren E.; Parvez, Masood; Rettig, Steven J.; Young, Victor G., Jr.
CS Department of Chemistry, University of Calgary, Calgary, AB, T2N 1N4, Can.
SO Organometallics (1999), 18(19), 3904-3912
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
OS CASREACT 131:271962
GI



I

AB Trimethylphosphine-stabilized ethylene complexes, e.g. I, of the ethylenebisindenyl-supported zirconocene fragment are prep'd. via magnesium redn. of rac-(EBI)ZrCl₂ in the presence of ethylene and PMe₃. When the reaction is halted after 6 h, good yields of a mixt. contg. rac-(EBI)Zr(.eta.2-CH₂:CH₂)PMe₃, rac-1, and the racemic diastereomer of the zirconacyclopentane deriv. (EBI)Zr(.eta.2-CH₂CH₂CH₂CH₂), rac-2, are obtained. This mixt. may be converted to pure rac-1 if treated with excess PMe₃. If the magnesium redn. of rac-(EBI)ZrCl₂ is left for 3 days in the presence of magnesium chloride, complete epimerization to meso-1 is obsd. Thus, both diastereomers of 1 are available. Compds. meso-1 and rac-2 have been characterized crystallog. The coordinated ethylene ligands in compds. 1 are susceptible to electrophilic attack by the pentafluorophenyl-substituted boranes HB(C₆F₅)₂ and B(C₆F₅)₃, forming zwitterionic metallocene products. For reactions involving HB(C₆F₅)₂, the products meso-3 and rac-3 are characterized by a strong zirconium-hydrido borate interaction, as well as a weak Zr-C.βeta. bonding. In addn. to complete soln. characterization, the structure of meso-3 was detd. crystallog. Upon treatment of rac-1 with B(C₆F₅)₃, a more charge-sepd. zwitterion, rac-4, was formed. In addn. to retaining

its PMe₃ ligand, the complex is stabilized by a strong .beta.-CH₂ interaction, as detd. by x-ray crystallog. and NMR spectroscopy. Structural comparisons between the compds. reported herein and previous examples in metallocene chem. are presented.

RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1996:170744 CAPLUS
DN 124:203315
TI Zwitterionic transition metal compounds, their preparation and use as olefin polymerization catalysts
IN Erker, Gerhard; Temme, Bodo; Aulbach, Michael; Bachmann, Bernd; Kueber, Frank
PA Hoechst A.-G., Germany
SO Ger. Offen., 10 pp.
CODEN: GWXXBX

DT Patent
LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 4420456	A1	19951214	DE 1994-4420456	19940613
	AU 9520278	A1	19951221	AU 1995-20278	19950524
	AU 691589	B2	19980521		
	EP 687682	A1	19951220	EP 1995-108411	19950601
	EP 687682	B1	20000119		
	R: AT, BE, DE, ES, FR, GB, IT, NL, SE				
	EP 992516	A2	20000412	EP 1999-110599	19950601
	EP 992516	A3	20021030		
	R: AT, BE, DE, ES, FR, GB, IT, NL, SE				
	ES 2142426	T3	20000416	ES 1995-108411	19950601
	TW 387905	B	20000421	TW 1995-84105602	19950605
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	US 6002032	A	19991214	US 1995-478900	19950607
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	NO 9502307	A	19951214	NO 1995-2307	19950612
	ZA 9504829	A	19960130	ZA 1995-4829	19950612
	BR 9502776	A	19960312	BR 1995-2776	19950612
	JP 08003212	A2	19960109	JP 1995-145881	19950613
	CN 1119648	A	19960403	CN 1995-107172	19950613
	CN 1069646	B	20010815		
PRAI	DE 1994-4420456	A	19940613		
	EP 1995-108411	A3	19950601		

OS MARPAT 124:203315

AB The zwitterionic compds. LnM+YZA-Rm [A = Group IB, IIB, III, IVA, V, VIB, VIIB, or VIIIB element; each L = .pi.-bonded ligand, electron donor (2 L may be joined by a bridging group); M = Group III-VI transition metal; each R = perhalocarbyl; Y = hetero atom, hydrocarbon residue; Z = hydrocarbon residue; m = 1-5, n = 1-4] are prep'd. by reaction of LnMX₂ (X = halogen) with YZ₂-, followed by treatment with ARm. Thus, [(dimethylsilylene)bis(2-methyl-4,5-benzindenyl)]zirconium dichloride and (2-butene-1,4-diyl)magnesium-2THF were stirred in toluene at -40.degree. and allowed to warm to room temp., filtered, and evapd. to dryness to give a red powder, which was redissolved in toluene and treated with tris(pentafluorophenyl)borane to give a zwitterion L₂Zr+CH₂CH:CHCH₂B-(C₆F₅)₃, where L₂ is the bridged bis(benzindenyl) ligand. This zwitterion, formed in situ, was used with iso-Bu₃Al to polymerize propylene, giving isotactic polypropylene with wt.-av. mol. wt. 298,000 and polydispersity 2.2. Other related zwitterions produced syndiotactic polypropylene.